

DERIVING FIXED BOND INFORMATION

ABSTRACT OF THE DISCLOSURE

Fixed bond information is derived. A fixed bond representation of a chemical structure is derived from a delocalized representation. A path is conceptually traced through the represented structure and an examination is conducted, for each atom, of each possible electronic and bonding state that is consistent with what has come before along the path. A result is found by extensively or exhaustively examining all possible states and orders in a semi-recursive procedure that is directed early towards likely answers. If there is more than one possible solution, the best solution is chosen by use of a rating function.

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